WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:37 PM GMT

|		
PDB ID	:	4PF1
Title	:	Crystal structure of aminopeptidase from marine sediment archaeon Thaumarchaeota archaeon
Authors	:	Michalska, K.; Chhor, G.; Fayman, K.; Endres, M.; Jedrzejczak, R.; Babnigg, G.; Steen, A.; Lloyd, K.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2014-04-25
Resolution	:	2.10 Å(reported)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
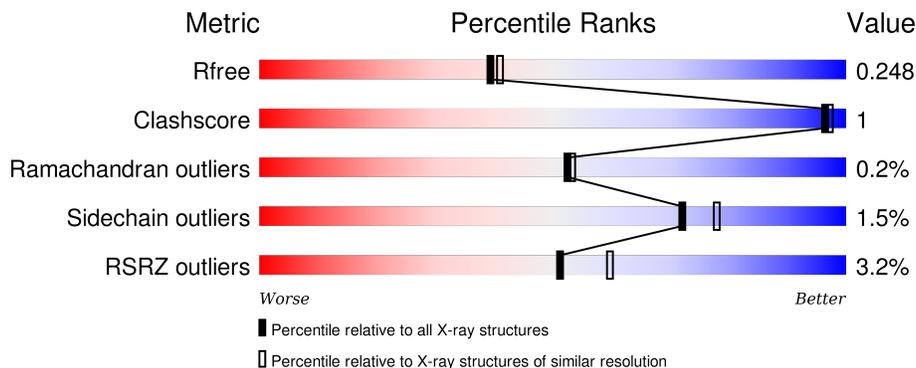
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	626	3% / 92% / 6% ·
1	B	626	3% / 92% / 5% ·
1	C	626	4% / 93% / 5% ·
1	D	626	3% / 92% / 5% ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PGE	D	706	-	-	-	X
3	GOL	A	702	-	-	-	X
3	GOL	A	703	-	-	-	X
3	GOL	A	704	-	-	-	X
3	GOL	A	705	-	-	-	X
3	GOL	B	702	-	-	-	X
3	GOL	B	704	-	-	-	X
3	GOL	C	701	-	-	-	X
3	GOL	D	703	-	-	-	X
3	GOL	D	704	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 20920 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Peptidase S15/CocE/NonD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	611	Total	C	N	O	S	0	3	0
			4938	3154	847	915	22			
1	B	610	Total	C	N	O	S	0	1	0
			4909	3138	838	910	23			
1	C	610	Total	C	N	O	S	0	0	0
			4901	3133	837	909	22			
1	D	611	Total	C	N	O	S	0	1	0
			4918	3143	842	911	22			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP M7TVE7
A	-1	ASN	-	expression tag	UNP M7TVE7
A	0	ALA	-	expression tag	UNP M7TVE7
B	-2	SER	-	expression tag	UNP M7TVE7
B	-1	ASN	-	expression tag	UNP M7TVE7
B	0	ALA	-	expression tag	UNP M7TVE7
C	-2	SER	-	expression tag	UNP M7TVE7
C	-1	ASN	-	expression tag	UNP M7TVE7
C	0	ALA	-	expression tag	UNP M7TVE7
D	-2	SER	-	expression tag	UNP M7TVE7
D	-1	ASN	-	expression tag	UNP M7TVE7
D	0	ALA	-	expression tag	UNP M7TVE7

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).
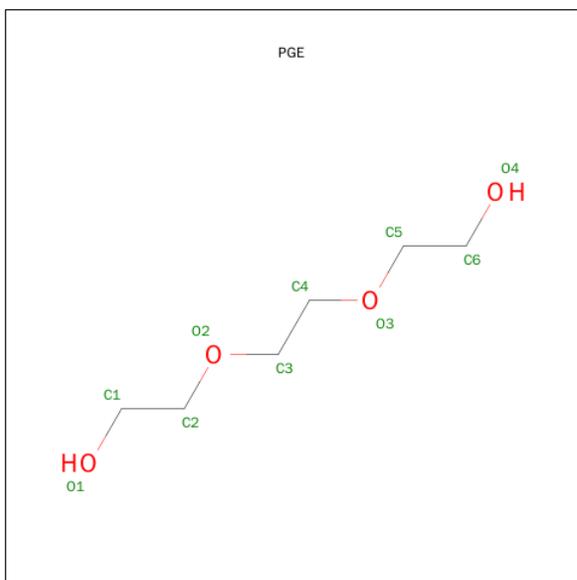
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 10	C 6	O 4		0	0
2	B	1	Total 10	C 6	O 4		0	0
2	D	1	Total 10	C 6	O 4		0	0
2	D	1	Total 10	C 6	O 4		0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
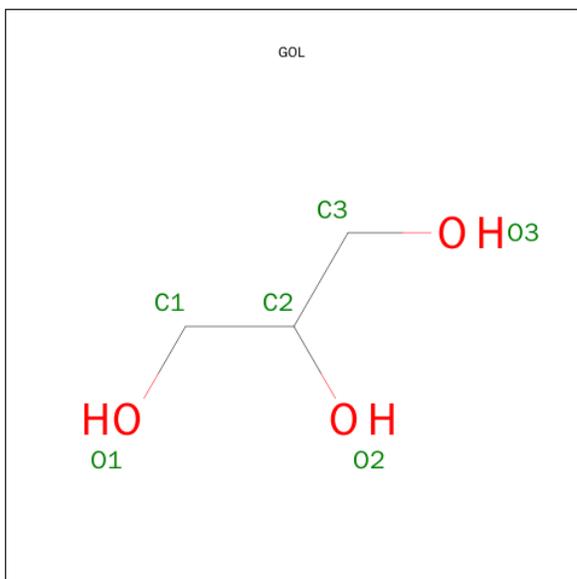
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	300	Total 300	O 300	0	0
4	B	287	Total 287	O 287	0	0
4	C	247	Total 247	O 247	0	0
4	D	290	Total 290	O 290	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Peptidase S15/CocE/NonD
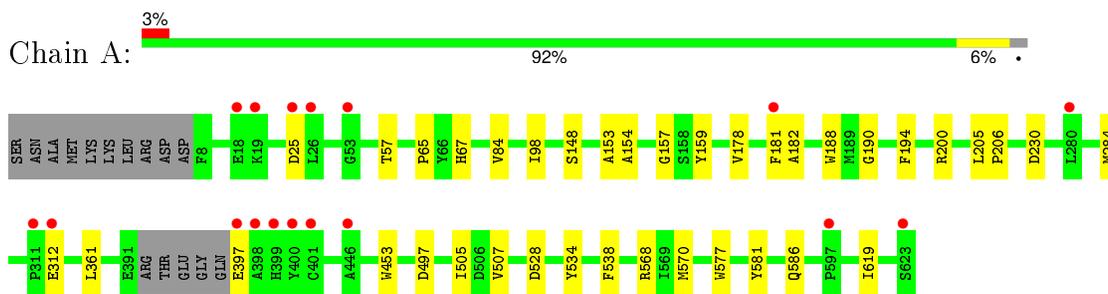
- Molecule 1: Peptidase S15/CocE/NonD
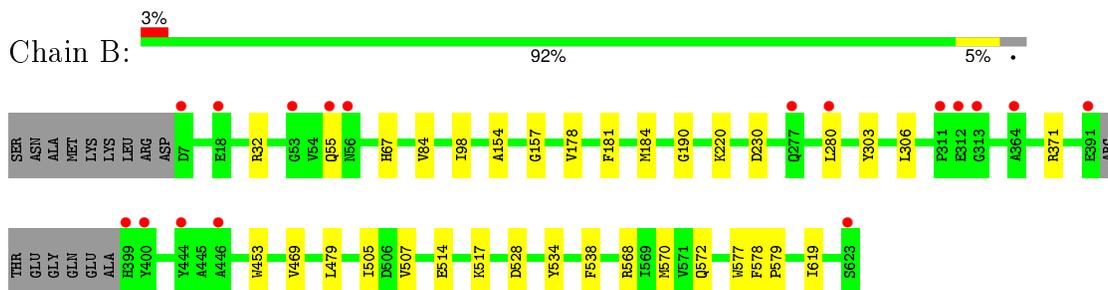
- Molecule 1: Peptidase S15/CocE/NonD
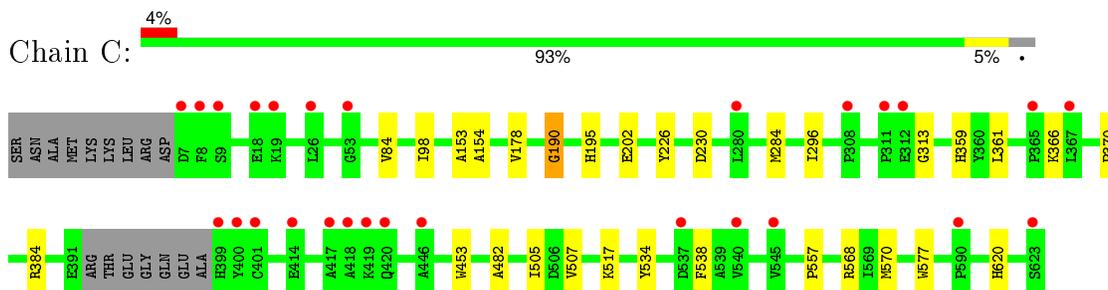
- Molecule 1: Peptidase S15/CocE/NonD
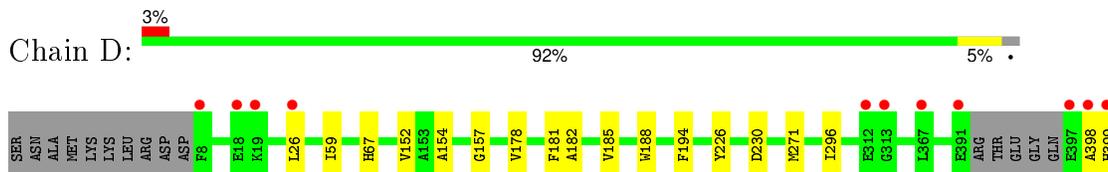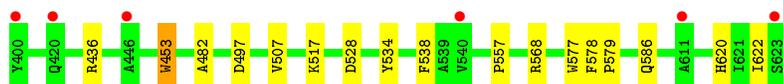
4 Data and refinement statistics (i)

| Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	118.43Å 108.14Å 120.38Å 90.00° 95.08° 90.00°	Depositor
Resolution (Å)	29.69 – 2.10 29.69 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.69-2.10) 99.6 (29.69-2.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.205 , 0.229 0.222 , 0.248	Depositor DCC
R_{free} test set	2166 reflections (1.25%)	DCC
Wilson B-factor (Å^2)	20.5	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 49.4	EDS
Estimated twinning fraction	0.020 for l,-k,h	Xtriage
L-test for twinning[2]	$< |L| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 175745 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	20920	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.66% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PGE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.43	0/5091	0.47	0/6935
1	B	0.42	0/5062	0.46	0/6897
1	C	0.42	0/5054	0.46	0/6887
1	D	0.42	0/5071	0.46	0/6909
All	All	0.42	0/20278	0.46	0/27628

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4938	0	4757	15	0
1	B	4909	0	4729	12	0
1	C	4901	0	4721	14	0
1	D	4918	0	4740	15	0
2	A	10	0	14	0	0
2	B	10	0	14	0	0
2	D	20	0	28	0	0
3	A	30	0	40	0	0
3	B	18	0	24	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	18	0	24	0	0
3	D	24	0	32	1	0
4	A	300	0	0	0	0
4	B	287	0	0	0	0
4	C	247	0	0	0	0
4	D	290	0	0	0	0
All	All	20920	0	19123	54	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (54) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:LYS:HD3	3:D:705:GOL:H12	1.85	0.58
1:C:84:VAL:HG11	1:C:98:ILE:HD13	1.90	0.53
1:D:534:TYR:HB3	1:D:538:PHE:HA	1.90	0.53
1:C:154:ALA:HB3	1:C:178:VAL:HG12	1.91	0.53
1:D:497:ASP:O	1:D:586:GLN:HA	2.10	0.52
1:C:507:VAL:HB	1:C:568:ARG:HB2	1.91	0.51
1:B:84:VAL:HG11	1:B:98:ILE:HD13	1.93	0.51
1:B:154:ALA:HB3	1:B:178:VAL:HG12	1.93	0.50
1:B:303:TYR:HE1	1:B:371:ARG:HD2	1.76	0.49
1:B:280:LEU:HD13	1:B:306:LEU:HD22	1.94	0.49
1:B:157:GLY:HA2	1:B:181:PHE:O	2.13	0.49
1:A:84:VAL:HG11	1:A:98:ILE:HD13	1.96	0.48
1:A:157:GLY:HA2	1:A:181:PHE:O	2.13	0.48
1:C:534:TYR:HB3	1:C:538:PHE:HA	1.95	0.48
1:D:188:TRP:HA	1:D:194:PHE:HB2	1.96	0.47
1:D:154:ALA:HB3	1:D:178:VAL:HG12	1.97	0.47
1:A:507:VAL:HB	1:A:568[A]:ARG:HB2	1.96	0.47
1:D:59:ILE:HB	1:D:152:VAL:HG22	1.96	0.46
1:C:370:PRO:HG3	1:C:384:ARG:HG2	1.97	0.46
1:C:359:HIS:CE1	1:C:366:LYS:HB2	2.51	0.45
1:C:178:VAL:HG23	1:C:284:MET:HG3	1.98	0.45
1:A:154:ALA:HB3	1:A:178:VAL:HG12	1.99	0.45
1:C:505:ILE:HB	1:C:570:MET:HB3	1.98	0.45
1:A:65:PRO:HG3	1:A:159:TYR:CD1	2.51	0.45
1:C:226:TYR:CZ	1:D:517:LYS:HA	2.52	0.44
1:D:482:ALA:O	1:D:620:HIS:HB3	2.18	0.44
1:B:184:MET:HB3	3:B:703:GOL:H12	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:482:ALA:O	1:C:620:HIS:HB2	2.17	0.44
1:A:178:VAL:HG23	1:A:284:MET:HG3	1.99	0.44
1:C:517:LYS:HA	1:D:226:TYR:CZ	2.53	0.44
1:D:185:VAL:HG13	1:D:271:MET:HB2	2.00	0.43
1:D:296:ILE:HG12	1:D:557:PRO:HB3	1.99	0.43
1:A:507:VAL:HB	1:A:568[B]:ARG:HB2	1.99	0.43
1:A:534:TYR:HB3	1:A:538:PHE:HA	2.00	0.43
1:B:534:TYR:HB3	1:B:538:PHE:HA	2.01	0.43
1:C:190:GLY:HA2	1:C:195:HIS:HA	2.01	0.43
1:C:153:ALA:HB2	1:C:361:LEU:HD11	2.00	0.43
1:D:157:GLY:HA2	1:D:181:PHE:O	2.19	0.43
1:B:469:VAL:HG22	1:B:572:GLN:HG2	1.99	0.43
1:C:296:ILE:HG12	1:C:557:PRO:HB3	2.01	0.43
1:A:153:ALA:HB2	1:A:361:LEU:HD11	2.01	0.42
1:D:436:ARG:HD2	1:D:453:TRP:HB2	2.01	0.42
1:A:505:ILE:HB	1:A:570:MET:HB3	2.01	0.42
1:A:188:TRP:HA	1:A:194:PHE:HB2	2.00	0.42
1:A:57:THR:O	1:A:148:SER:HA	2.19	0.42
1:D:398:ALA:HB2	1:D:622:ILE:HG22	2.01	0.42
1:B:505:ILE:HB	1:B:570:MET:HB3	2.01	0.42
1:A:200:ARG:HG3	1:A:581:TYR:CE2	2.55	0.42
1:B:507:VAL:HB	1:B:568:ARG:HB2	2.02	0.41
1:D:507:VAL:HB	1:D:568:ARG:HB2	2.02	0.41
1:D:578:PHE:CG	1:D:579:PRO:HA	2.56	0.41
1:A:497:ASP:O	1:A:586:GLN:HA	2.21	0.41
1:B:578:PHE:CG	1:B:579:PRO:HA	2.56	0.41
1:A:205:LEU:HB2	1:A:206:PRO:HD3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	610/626 (97%)	588 (96%)	20 (3%)	2 (0%)	46	45
1	B	607/626 (97%)	583 (96%)	23 (4%)	1 (0%)	52	53
1	C	606/626 (97%)	578 (95%)	26 (4%)	2 (0%)	46	45
1	D	608/626 (97%)	582 (96%)	25 (4%)	1 (0%)	52	53
All	All	2431/2504 (97%)	2331 (96%)	94 (4%)	6 (0%)	52	53

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	190	GLY
1	C	313	GLY
1	A	182	ALA
1	D	182	ALA
1	A	190	GLY
1	B	190	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	526/536 (98%)	517 (98%)	9 (2%)	68	74
1	B	524/536 (98%)	513 (98%)	11 (2%)	61	66
1	C	523/536 (98%)	519 (99%)	4 (1%)	86	91
1	D	524/536 (98%)	517 (99%)	7 (1%)	76	82
All	All	2097/2144 (98%)	2066 (98%)	31 (2%)	72	78

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ASP
1	A	67	HIS
1	A	230	ASP
1	A	312	GLU
1	A	397	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	453	TRP
1	A	528	ASP
1	A	577	TRP
1	A	619	ILE
1	B	32	ARG
1	B	55	GLN
1	B	67	HIS
1	B	230	ASP
1	B	453	TRP
1	B	479	LEU
1	B	514	GLU
1	B	517	LYS
1	B	528	ASP
1	B	577	TRP
1	B	619	ILE
1	C	202	GLU
1	C	230	ASP
1	C	453	TRP
1	C	577	TRP
1	D	26	LEU
1	D	67	HIS
1	D	230	ASP
1	D	399	HIS
1	D	453	TRP
1	D	528	ASP
1	D	577	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	437	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

19 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	PGE	A	701	-	9,9,9	0.12	0	8,8,8	0.06	0
3	GOL	A	702	-	5,5,5	0.13	0	5,5,5	0.19	0
3	GOL	A	703	-	5,5,5	0.12	0	5,5,5	0.18	0
3	GOL	A	704	-	5,5,5	0.14	0	5,5,5	0.25	0
3	GOL	A	705	-	5,5,5	0.13	0	5,5,5	0.30	0
3	GOL	A	706	-	5,5,5	0.12	0	5,5,5	0.19	0
2	PGE	B	701	-	9,9,9	0.12	0	8,8,8	0.06	0
3	GOL	B	702	-	5,5,5	0.15	0	5,5,5	0.19	0
3	GOL	B	703	-	5,5,5	0.12	0	5,5,5	0.25	0
3	GOL	B	704	-	5,5,5	0.13	0	5,5,5	0.30	0
3	GOL	C	701	-	5,5,5	0.12	0	5,5,5	0.17	0
3	GOL	C	702	-	5,5,5	0.14	0	5,5,5	0.16	0
3	GOL	C	703	-	5,5,5	0.12	0	5,5,5	0.18	0
2	PGE	D	701	-	9,9,9	0.13	0	8,8,8	0.06	0
3	GOL	D	702	-	5,5,5	0.12	0	5,5,5	0.34	0
3	GOL	D	703	-	5,5,5	0.12	0	5,5,5	0.18	0
3	GOL	D	704	-	5,5,5	0.13	0	5,5,5	0.27	0
3	GOL	D	705	-	5,5,5	0.13	0	5,5,5	0.25	0
2	PGE	D	706	-	9,9,9	0.14	0	8,8,8	0.06	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PGE	A	701	-	-	0/7/7/7	0/0/0/0

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	702	-	-	0/4/4/4	0/0/0/0
3	GOL	A	703	-	-	0/4/4/4	0/0/0/0
3	GOL	A	704	-	-	0/4/4/4	0/0/0/0
3	GOL	A	705	-	-	0/4/4/4	0/0/0/0
3	GOL	A	706	-	-	0/4/4/4	0/0/0/0
2	PGE	B	701	-	-	0/7/7/7	0/0/0/0
3	GOL	B	702	-	-	0/4/4/4	0/0/0/0
3	GOL	B	703	-	-	0/4/4/4	0/0/0/0
3	GOL	B	704	-	-	0/4/4/4	0/0/0/0
3	GOL	C	701	-	-	0/4/4/4	0/0/0/0
3	GOL	C	702	-	-	0/4/4/4	0/0/0/0
3	GOL	C	703	-	-	0/4/4/4	0/0/0/0
2	PGE	D	701	-	-	0/7/7/7	0/0/0/0
3	GOL	D	702	-	-	0/4/4/4	0/0/0/0
3	GOL	D	703	-	-	0/4/4/4	0/0/0/0
3	GOL	D	704	-	-	0/4/4/4	0/0/0/0
3	GOL	D	705	-	-	0/4/4/4	0/0/0/0
2	PGE	D	706	-	-	0/7/7/7	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	703	GOL	1	0
3	D	705	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	611/626 (97%)	0.13	17 (2%)	56	64	9, 20, 36, 69	0
1	B	610/626 (97%)	0.18	17 (2%)	56	64	11, 22, 38, 61	0
1	C	610/626 (97%)	0.32	27 (4%)	38	47	13, 25, 44, 69	0
1	D	611/626 (97%)	0.15	17 (2%)	56	64	13, 22, 39, 68	0
All	All	2442/2504 (97%)	0.20	78 (3%)	51	60	9, 22, 40, 69	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	398	ALA	5.9
1	C	418	ALA	5.5
1	B	446	ALA	5.2
1	C	311	PRO	4.6
1	D	397	GLU	4.4
1	B	53	GLY	3.9
1	A	399	HIS	3.8
1	A	446	ALA	3.8
1	A	311	PRO	3.7
1	B	312	GLU	3.6
1	B	55	GLN	3.6
1	C	308	PRO	3.5
1	D	399	HIS	3.5
1	D	26	LEU	3.4
1	C	417	ALA	3.3
1	A	398	ALA	3.3
1	D	400	TYR	3.3
1	D	18	GLU	3.3
1	A	312	GLU	3.2
1	A	18	GLU	3.2
1	B	399	HIS	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	400	TYR	3.1
1	C	7	ASP	3.1
1	D	420	GLN	3.1
1	A	397	GLU	3.0
1	C	399	HIS	3.0
1	B	7	ASP	2.9
1	A	400	TYR	2.9
1	D	8	PHE	2.9
1	A	53	GLY	2.9
1	D	19	LYS	2.9
1	B	280	LEU	2.9
1	C	419	LYS	2.9
1	C	312	GLU	2.9
1	C	540	VAL	2.9
1	A	19	LYS	2.9
1	B	364	ALA	2.9
1	C	8	PHE	2.8
1	A	401	CYS	2.8
1	B	311	PRO	2.8
1	D	391	GLU	2.8
1	C	18	GLU	2.7
1	D	623	SER	2.7
1	A	623	SER	2.7
1	C	400	TYR	2.7
1	C	446	ALA	2.6
1	C	26	LEU	2.6
1	B	277	GLN	2.6
1	B	18	GLU	2.6
1	C	420	GLN	2.5
1	A	280	LEU	2.5
1	B	313	GLY	2.5
1	C	280	LEU	2.5
1	A	25	ASP	2.5
1	B	444	TYR	2.4
1	D	312	GLU	2.4
1	B	623	SER	2.4
1	D	540	VAL	2.4
1	D	611	ALA	2.4
1	A	26	LEU	2.4
1	D	446	ALA	2.3
1	C	545	VAL	2.3
1	C	623	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	9	SER	2.3
1	A	597	PRO	2.3
1	C	590	PRO	2.3
1	C	53	GLY	2.2
1	B	391	GLU	2.2
1	C	414	GLU	2.2
1	D	313	GLY	2.2
1	C	19	LYS	2.1
1	C	367	LEU	2.1
1	C	401	CYS	2.1
1	B	56	ASN	2.0
1	C	537	ASP	2.0
1	D	367	LEU	2.0
1	A	181	PHE	2.0
1	C	365	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	GOL	D	703	6/6	0.88	0.19	12.21	40,42,43,43	0
3	GOL	A	702	6/6	0.91	0.28	11.87	28,29,30,31	0
3	GOL	D	704	6/6	0.79	0.24	6.06	31,33,33,34	0
3	GOL	B	704	6/6	0.85	0.22	5.16	29,30,30,31	0
3	GOL	A	704	6/6	0.87	0.19	4.76	31,34,36,38	0
3	GOL	A	705	6/6	0.86	0.20	4.43	26,28,29,29	0

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
3	GOL	C	701	6/6	0.86	0.22	3.95	43,43,43,44	0
3	GOL	B	702	6/6	0.91	0.16	3.58	22,28,31,32	0
3	GOL	A	703	6/6	0.91	0.18	2.55	29,31,32,33	0
2	PGE	D	706	10/10	0.85	0.20	2.13	41,43,46,46	0
3	GOL	C	702	6/6	0.87	0.14	1.95	29,32,32,32	0
3	GOL	B	703	6/6	0.92	0.17	1.61	31,32,33,34	0
2	PGE	B	701	10/10	0.93	0.12	1.22	28,29,30,31	0
3	GOL	D	702	6/6	0.92	0.13	1.02	26,28,30,30	0
2	PGE	A	701	10/10	0.82	0.16	0.91	44,46,49,49	0
2	PGE	D	701	10/10	0.91	0.09	-0.18	31,33,36,36	0
3	GOL	C	703	6/6	0.79	0.19	-	40,41,42,42	0
3	GOL	A	706	6/6	0.92	0.26	-	46,46,47,48	0
3	GOL	D	705	6/6	0.86	0.28	-	39,40,41,41	0

6.5 Other polymers (i)

There are no such residues in this entry.